Review of reaction datasets available

This review aims to present the reaction datasets available in the ORD and give a short description of the chemistry they are studying. Making it easy to estimate the chemical space explored in each of them.

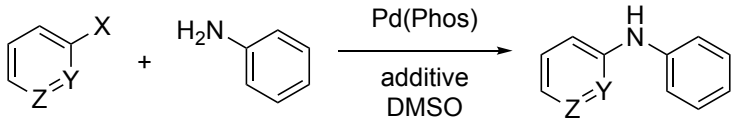
1 HTE - Screenings :

1.1 hte_ahneman :

The Ahneman dataset is a well known HTE dataset.[1]

It is available in the ORD : data/46/ord_dataset-46ff9a32d9e04016b9380b1b1ef949c3.pb.gz

Number of reactions	Number of variables
4312	Ligand : 4, Bases : 3, Additives : 23, Ar_halides : 15

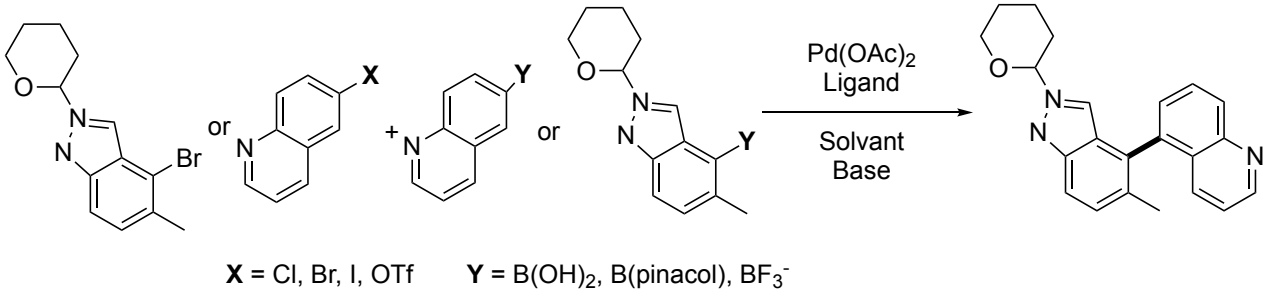


1.2 hte_perera :

The Perera dataset is a well known HTE dataset.[6]

It is available in the ORD : 'data/68/ord_dataset-68cb8b4b2b384e3d85b5b1efae58b203.pb.gz'

Number of reactions	Number of variables
5760	Ar_halide :5, solvents :4, Ligand_in_solvent :(12x2), Base_in_solvent :(8x4), Boronate_in_solvent (8x3)

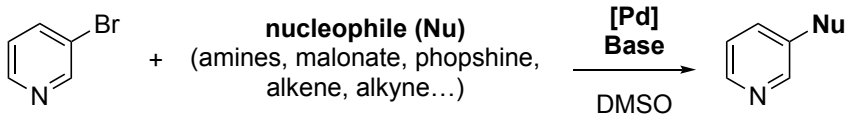


1.3 hte_santanilla :

The Santanilla dataset is a HTE dataset of a Pd cross coupling.[2]

It is available in the ORD : 'data/7d/ord_dataset-7d8f5fd922d4497d91cb81489b052746.pb.gz'

Number of reactions	Number of variables
1536	Catalyst (16), Nucleophiles (16), Bases (6)



1.4 hte_dreher :

1.4.1 dreher_hte cheminformers library :

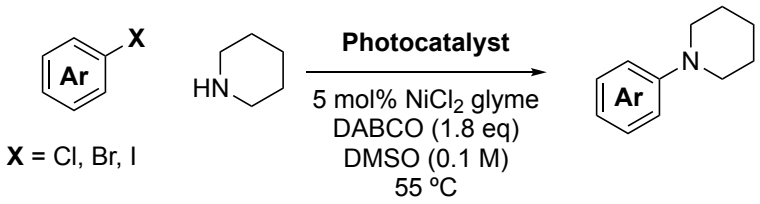
The Dreher dataset is a HTE dataset build in order to make cheminformers library for reaction benchmark, the data comes from experiment 2 presented in SI.[3]

The susbtrates are complex molecules of pharmaceutical interest (Ar-X, X = Cl, Br or I).

Not sure whether the SI experiment 1 is available or not but it is interesting as it is a kind of HTE optimization (48x32 = 1536 reactions) and exp. 2 is more like an HTE scope (1728 reactions).

It is available in the ORD : 'data/ac/ord_dataset-ac78456835404910b3a4c840248b6ac9.pb.gz'

Number of reactions	Number of variables
1728	Photocatalyst (11, amount :4), Ar-X (18), Piperidine (amount :2), Photocatalyst_2 (2 = one or nothing)



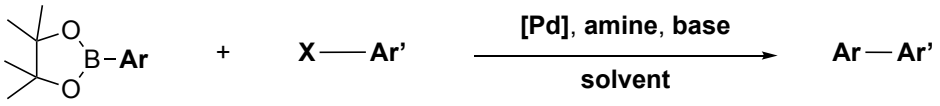
1.4.2 dreher_first cheminformers library :

The Dreher dataset is a HTE dataset build in order to make cheminformers library for reaction benchmark, the data comes from experiment 2 presented in SI.[4]

first 8 rows of Figure 4D

It is available in the ORD : 'data/ac/ord_dataset-ac78456835404910b3a4c840248b6ac9.pb.gz'

Number of reactions	Number of variables
264	boronate (24), aryl halides (18), Catalyst (8), Solvent (6), Bases(7), indole_halide (additive : 3), Base_2 (3)



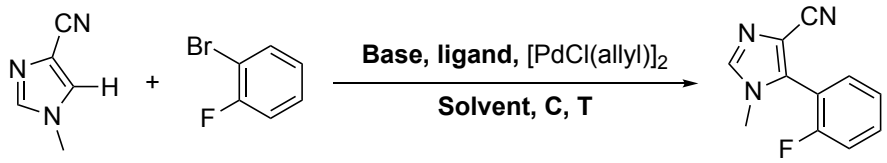
There are additionnal data on :
— cyanation methods of the pinacols boronates
— aryl halide CN coupling methods (Pd or Cu).

1.5 hte_shields :

The Shield HTE dataset is a direct arylation presented in order to benchmark the EDBO for reaction design.[8]
This dataset is constituted of one first full HTE dataset presented below and of an extended dataset constituted of the ful HTE screening for 2 new ligands, all others parameters varying (256/288 possible reactions performed).

It was downloaded from the EDBO git :https://github.com/b-shields/edbo

Number of reactions	Number of variables
1728	Ligands (12), Bases (4), Solvent (4), Concentrations(3) and Temperatures (3)

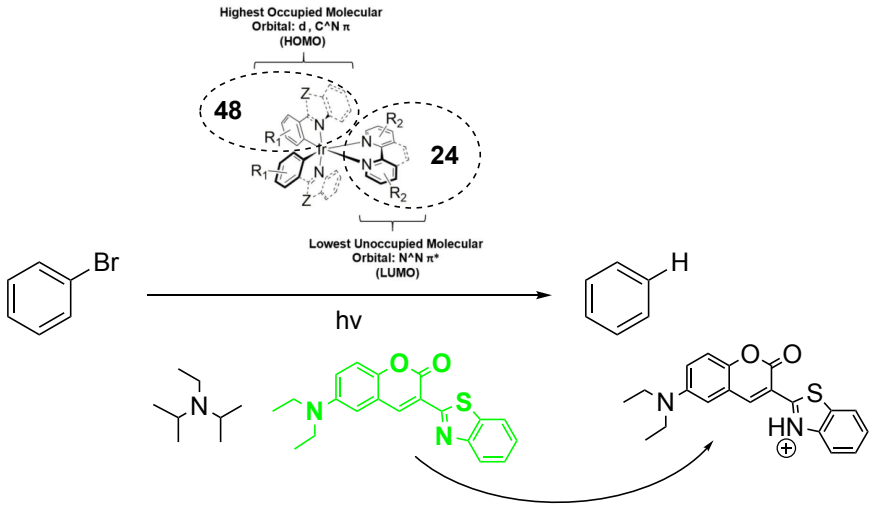


1.6 hte_photo :

The photo dataset is a HTE dataset build in order to screen Ir photocatalyst detailed below, for the dehalogenation of Ar-Br compounds. The output meausured is the conversion obtained after a certain time by UV-vis spectroscopy which considerably ease the analysis process.[5]
The only reaction parameter is the Ir(III) photo catalyst

It is available in the ORD : 'data/b4/ord_dataset-b440f8c90b6343189093770060fc4098.pb.gz'

Number of reactions	Number of variables
1152	Photocatalyst (1152 = 48x24)

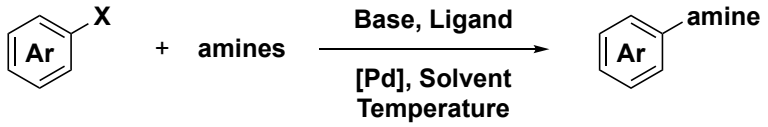


2 ELN :

The only ELN dataset available in the one of the preprint of Saebi.[7]
It is available in the ORD : 'data/00/ord_dataset-00005539a1e04c809a9a78647bea649c.pb.gz'

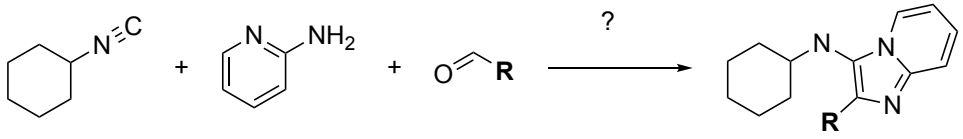
Number of reactions	Number of variables
750	Bases (13), Ligands (24), Catalyst (12), Ar-X (298), Amines (233), temperature (28), solvent (16)

For each reaction parameter the amount in moles and the solvent volume is detailed.



3 Imidazole :

A scope of multicomponent reactions. No reference given in the ORD.
It is available in the ORD : 'data/10/ord_dataset-10b940e7982c4622b1e1ac879394aba6.pb.gz'
384 aldéhydes for 384 reactions.

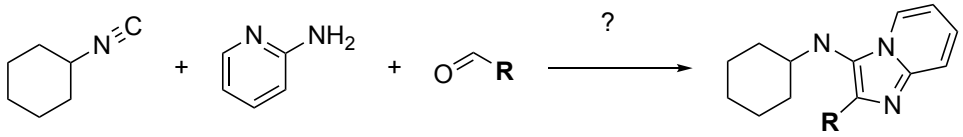


4 Suzuki Experiment :

Cliff activity for phosphines. (Newmann2021).
It is available in the ORD : 'data/3b/ord_dataset-3b5db90e337942ea886b8f5bc5e3aa72.pb.gz'

Number of reactions	Number of variables
450	Ar-Cl (2), ArB(OH)2 (5), ligands (90)

For each reaction parameter the amount in moles and the solvent volume is detailed.



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